A covering property of Hofstadter's butterfly

R. Ketzmerick,[1,2] K. Kruse,[1] F. Steinbach,[1] and T. Geisel[1]

[1] Max-Planck-Institut für Strömungsforschung und Institut für Nichtlineare Dynamik der Universität Göttingen, Bunsenstr. 10, D-37073 Göttingen, Germany

[2] Physics Department and Institute for Theoretical Physics, UCSB, Santa Barbara, California 93106

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Based on a thorough numerical analysis of the spectrum of Harper's operator, which describes, e.g., an electron on a two-dimensional lattice subjected to a magnetic field perpendicular to the lattice plane, we make the following conjecture: For any value of the incommensurability parameter σ of the operator its spectrum can be covered by the bands of the spectrum for every rational approximant of σ after stretching them by factors with a common upper bound. We show that this conjecture has the following important consequences: For *all* irrational values of σ the spectrum is (i) a zero measure Cantor set and has (ii) a Hausdorff dimension less or equal to 1/2. We propose that our numerical approach may be a guide in finding a rigorous proof of these results.

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I. INTRODUCTION

The Harper model [1] may be considered as the most important system in the realm of quasi-periodic systems. It is described by the one-dimensional tight-binding Hamiltonian

$$H_{\lambda,\sigma,\nu} = \sum_n a_{n+1}^\dagger a_n + a_{n-1}^\dagger a_n + \lambda \cos(2\pi\sigma n + \nu) a_n^\dagger a_n,$$
(1)

where λ, σ, and ν are real valued parameters, and $a_n^\dagger$ and a_n are creation and annihilation operators at site n. Depending on whether σ is rational or irrational this Hamiltonian is periodic or quasi-periodic, resp. The model exhibits rich spectral features which showed up for the first time in the numerical work of Hofstadter [2] who computed its spectrum for $\lambda = 2$ as a function of σ. The beautiful resulting graph (Fig. 1) is today known as Hofstadter's butterfly and has attracted a lot of attention among physicists and mathematicians ever since.

From a physical point of view the Harper model was first introduced to describe electrons moving in a two-dimensional periodic potential with a square unit cell and subjected to a weak magnetic field perpendicular to the potential plane [1–4]. In this case, Harper's model describes the eigenfunctions in one direction of the underlying Bravais lattice after separating plane waves in the perpendicular direction. Then, the parameter λ is twice the ratio of the modulation amplitudes in these two directions, σ is given by the number of magnetic flux quanta per unit cell of the potential, and ν is the wave number of the plane wave being separated. Such a system can be realized, e.g., by lateral superlattices on semiconductor heterostructures in which the first experimental indications of Hofstadter's butterfly were found recently [5]. Harper's model also appeared in the opposite limit, namely for electrons in a two-dimensional periodic potential with strong magnetic field [6], as well as in other physical contexts, e.g., phonons in a quasi-periodic potential [7] and superconducting networks [8]. Apart from describing real physical systems it is an important and simple model exhibiting a metal-insulator transition [9]: if σ is a typical irrational, then for $\lambda < 2$ all eigenfunctions are extended while for $\lambda > 2$ they are localized. Hence, at $\lambda = 2$ a metal-insulator transition occurs and unusual properties of the spectrum and the eigenfunctions are expected. This has led mathematicians to study Harper's model as a simple example of a system with a possibly singular continuous spectrum. In particular, at $\lambda = 2$ the spectrum has been conjectured to be a zero measure Cantor set for irrational values of σ [2,10]. This has been shown for a large class of irrationals by Helffer and Sjöstrand [11] and Last [12], which, however, do not cover the irrationals typically used in numerical investigations, namely irrationals with bounded continued fraction expansions, e.g., the Golden Mean $(\sqrt{5}-1)/2$. So still the question remains whether the spectrum is a zero measure Cantor set for *all* irrational values of σ [13,14].

For both, physicists and mathematicians, the Harper model is also an important example for the study of the relation between the spectral properties and the dynamics of quantum systems [15–21]. In 1988, Hiramoto and Abe numerically discovered anomalous diffusive spreading of wave packets in the Harper model for $\lambda = 2$ [15]. Furthermore, the model has been used for testing relations proposed between the fractal properties of the spectral measure and the temporal decay of autocorrelations [16] as well as for the asymptotic growth of the moments of a wave packet [18,20,21]. In these studies one is thus interested in fractal properties of the spectrum, the easiest being the Hausdorff dimension. First, it was investigated numerically [18,22–24] and recently a perturbative calculation has been presented for σ the Golden and the Silver Mean [25]. For a class of irrationals, which has zero Lebesgue measure, Last proved the Hausdorff dimension to be bounded from above by 1/2 [12]. It remains open whether this bound is valid for *all* irrationals.

In this article we study the operator (1) at the critical point $\lambda = 2$. Based on a numerical analysis we present our conjecture that there is a constant R such that the spectrum for any value of σ can be covered by the q bands of the spectrum for any rational approximant p/q of σ after stretching each of these bands by a factor smaller than R. This conjecture permits us to prove for *all* irrational σ that the spectrum is (i) a zero measure Cantor set and has (ii) a Hausdorff dimension less or equal to $1/2$. After presenting the relevant basic facts on Harper's operator in Sec. II, in Sec. III we precisely state our conjecture and deduce the above mentioned statements on the measure of the spectrum and its Hausdorff dimension. Section IV contains a thorough numerical analysis of Hofstadter's butterfly substantiating the validity of our conjecture.

II. BASIC FACTS

In the following we review the facts about the spectrum of Harper's operator [Eq. (1)] that are used in the proofs presented in Sec. III. The relevant energy spectrum $S(\sigma)$ of the Harper model for $\lambda = 2$ and a fixed value of σ is given by the set

$$S(\sigma) \equiv \bigcup_\nu Spec\left(H_{2,\sigma,\nu}\right), \qquad (2)$$

where $Spec\left(H_{2,\sigma,\nu}\right)$ denotes the spectrum of $H_{2,\sigma,\nu}$. Figure 1 shows $S(\sigma)$ vs. σ, the so-called Hofstadter butterfly [2], revealing its symmetries with respect to $E = 0$ and $\sigma = 1/2$.

For rational $\sigma = p/q$, with p and q relatively prime, the operator (1) is periodic and $S(\sigma)$ consists of q bands. These bands are separated by $q - 1$ gaps in the case of q odd and $q - 2$ gaps for q even, for which the middle bands touch each other at $E = 0$ [27]. The Lebesgue measure $|S(p/q)|$ of the spectrum obeys [12]

$$\frac{2(\sqrt{5}+1)}{q} < \left|S\left(\frac{p}{q}\right)\right| < \frac{8e}{q}, \qquad (3)$$

where $e = \exp(1) = 2,71\ldots$.

For irrational values of σ, the operator (1) is quasi-periodic and its spectrum contains no isolated points as follows from general results on ergodic Jacobi matrices [28]. Furthermore, it is independent of ν [28], such that $S(\sigma)$ is a closed set. Thus, if $S(\sigma)$ has measure zero it will be nowhere dense and therefore will be a Cantor set. As the measure $|S(p/q)|$ of rational approximants p/q of σ decreases to zero with increasing q [Eq. (3)], one may naively think that indeed $|S(\sigma)| = 0$ holds. *Rigorously*, however, $|S(\sigma)|$ can only be shown to vanish for two classes of irrationals σ: One class consists of the irrationals for which all coefficients in the continued fraction expansion are larger than some constant [11], while the irrationals in the other class have an unbounded continued

fraction expansion [12]. The latter proof uses a continuity property of the spectrum, namely that the spectrum $S(\sigma)$ is Hölder continuous of order $1/2$ [26], i.e., for every eigenvalue E in the spectrum for σ there is a nearby eigenvalue E' in the spectrum for σ' with

$$\left|E - E'\right| \leq 6(2|\sigma - \sigma'|)^{1/2}. \qquad (4)$$

This allows to construct a sequence of covers of $S(\sigma)$ using the approximants $\{p_n/q_n\}_{n=0}^\infty$ of the continued fraction expansion of σ. For each n one attaches intervals of length $6(2|\sigma - p_n/q_n|)^{1/2}$ to each of the $2q_n$ band edges of $S(p_n/q_n)$. According to Eq. (4) this defines a cover $S_{q_n}(\sigma)$ of $S(\sigma)$ consisting of q_n intervals. The measure of any of these covers is

$$S_{q_n}(\sigma) = \left|S\left(\frac{p_n}{q_n}\right)\right| + 12q_n\left(2\left|\sigma - \frac{p_n}{q_n}\right|\right)^{1/2} \qquad (5)$$

$$< \frac{8e}{q_n} + 12q_n\left(2\left|\sigma - \frac{p_n}{q_n}\right|\right)^{1/2} \qquad (6)$$

by Eq. (3). For $n \to \infty$ the measure vanishes only if $\lim_{n\to\infty} q_n^2|\sigma - p_n/q_n| = 0$, which is fulfilled for irrationals with an unbounded continued fraction expansion and proves a zero measure Cantor set spectrum for these irrationals [12]. For general σ, which fulfill

$$\left|\sigma - \frac{p}{q}\right| \leq \frac{C}{q^2}, \qquad (7)$$

for some constant $C > 0$, covers as described above do not permit to show $|S(\sigma)| = 0$. With respect to the Hausdorff dimension these covers have been used by Last [12] to show an upper bound of $1/2$ for the zero measure set of irrationals fulfilling $q_n^4|\sigma - p_n/q_n| < \tilde{C}$ for all n and some constant $\tilde{C} > 0$. In the following, we will present a conjecture, stating that there is a useful cover obtained by stretching the bands of a rational approximant of σ. Assuming this conjecture we prove that the Lebesgue measure of the spectrum is zero as well as that its Hausdorff dimension is less or equal to $1/2$ for *all* irrationals.

III. THE CONJECTURE AND ITS IMPLICATIONS

In this section we will show how the zero measure Cantor structure of spectra for irrational values of σ and an upper bound of their Hausdorff dimension follow from our

Conjecture 1 : *There is a constant $R > 0$ such that for any irrational $\sigma \in [0,1]$ and any two rational approximants p/q and p'/q' with $q < q'$, which are obtained by truncating the continued fraction expansion of σ, there exists a cover $S_q(p'/q')$ of $S(p',q')$ consisting of q intervals with the property*

$$\left|S_q\left(\frac{p'}{q'}\right)\right| \leq R\left|S\left(\frac{p}{q}\right)\right|. \qquad (8)$$

2

Before giving the explicit construction of such a cover and numerically substantiating this Conjecture in the next section, we will now discuss its consequences. One can replace p'/q' in Eq. (8) by an irrational σ as is stated in **Corollary 1 :** *Assuming Conjecture 1, there is a constant $R > 0$ such that for any irrational $\sigma \in [0, 1]$ and any rational approximant p/q obtained by truncating the continued fraction expansion of σ there exists a cover $\tilde{S}_q(\sigma)$ of $S(\sigma)$ consisting of q intervals with the property*

$$\left| \tilde{S}_q(\sigma) \right| < \frac{8eR + 1}{q}. \tag{9}$$

Proof: Let σ be an irrational and let p/q be a rational approximant of σ, which is obtained by truncating its continued fraction expansion. Then, one can always choose a sufficently high rational approximant p'/q' of σ, which again is obtained by truncating its continued fraction expansion, such that

$$q' \geq 12q^2\sqrt{2C}, \tag{10}$$

where C is the constant of Eq. (7). We now define a q-cover $\tilde{S}_q(\sigma)$ of the spectrum for σ using the continuity property Eq. (4). To this end we take the q intervals of the cover $S_q(p'/q')$, as given by Conjecture 1, and enlarge them by $6(2|\sigma - (p'/q')|)^{1/2}$ at the lower and upper ends, respectively. For the Lebesgue measure $|\tilde{S}_q(\sigma)|$ of $\tilde{S}_q(\sigma)$ we thus have

$$\left| \tilde{S}_q(\sigma) \right| \leq \left| S_q\left(\frac{p'}{q'}\right) \right| + 2q \cdot 6\left(2\left|\sigma - \frac{p'}{q'}\right|\right)^{1/2} \tag{11}$$

$$\leq \left| S_q\left(\frac{p'}{q'}\right) \right| + 12\sqrt{2C}\,\frac{q}{q'} \tag{12}$$

$$\leq \left| S_q\left(\frac{p'}{q'}\right) \right| + \frac{1}{q}, \tag{13}$$

where we have used Eq. (7). Finally, using Conjecture 1 and Eq. (3) we obtain Eq. (9). $\square$

From this Corollary follows
Theorem 1 : *Assuming Conjecture 1, for any irrational $\sigma \in [0, 1]$ the set $S(\sigma)$ is of zero Lebesgue measure. Proof*: By taking the limit $q \to \infty$ in Eq. (9) this follows immediately. $\square$

The Cantor structure of the spectrum for irrational σ is a direct consequence of Theorem 1 and stated in
Corollary 2 : *Assuming Conjecture 1, for any irrational $\sigma \in [0, 1]$ the set $S(\sigma)$ is a Cantor set. Proof*: Since the spectrum $S(\sigma)$ is closed, Theorem 1 shows that it is nowhere dense. As it is also known to have no isolated points [28], it follows that $S(\sigma)$ is a Cantor set. $\square$

As a second application of Conjecture 1, we now give an upper bound on the Hausdorff dimension D_H of the spectrum. Most of the proof is contained in
Lemma 2 (Ref. [12])**:** *Let $S \subset \mathbb{R}$, and suppose that S has a sequence of covers: $\{S_{q_n}\}_{n=1}^{\infty}$, $S \subset S_{q_n}$, such that*

each S_{q_n} is a union of q_n intervals, $q_n \to \infty$ as $n \to \infty$, and for each n:

$$|S_{q_n}| < \frac{c}{q_n^{\beta}}, \tag{14}$$

where β and c are positive constants; then:

$$D_H(S) \leq \frac{1}{1 + \beta}. \tag{15}$$

Proof: See Ref. [12].

Theorem 2 : *Assuming Conjecture 1, for any irrational $\sigma \in [0, 1]$ we have*

$$D_H\big(S(\sigma)\big) \leq \frac{1}{2}. \tag{16}$$

Proof: Choosing for S_{q_n} in Lemma 1 a cover satisfying Eq.(9) of Corollary 1 and then comparing Eqs. (9) and (14) yields $\beta = 1$. Inserting this into Eq. (15) concludes the proof of Theorem 2. $\square$

IV. THE COVER

In this section we present a specific cover which is numerically shown to satisfy Conjecture 1. A good starting point for covering the spectrum of Harper's operator [Eq. (1)] for some rational σ' are the bands of the spectrum for a rational σ obtained by truncating the continued fraction expansion of σ'. In fact, there is a natural assignment of any of these bands to a cluster of bands of the spectrum for σ', which is determined by Hofstadter's Rules (see Appendix). Very often a band is too narrow to cover its related cluster, e.g., the lowest band of $\sigma = 1/3$ does not cover the related cluster consisting of the lowest two bands for $\sigma' = 2/5$. Therefore, we introduce the factor $R_i(\frac{p}{q}, \frac{p'}{q'})$ by which the i-th band, $i = 1, 2, \ldots, q$, of the spectrum for $\sigma = p/q$ has to be stretched in order to cover its related cluster of the spectrum for $\sigma' = p'/q'$.

We numerically analyzed the stretching factors R_i for all allowed pairs p/q and p'/q' with $q' \leq 300$ and found that they are bounded from above by

$$\max_{\substack{p,q,p',q',i \\ q' \leq 300}} R_i\left(\frac{p}{q}, \frac{p'}{q'}\right) \leq 2.1 \quad . \tag{17}$$

If a bound would exist *without* the restriction $q' \leq 300$ for any two rational approximants p/q and p'/q' with $q < q'$, that are obtained by truncating the continued fraction expansion of some irrational $\sigma \in [0, 1]$, then the cover described above would fulfill Conjecture 1. In the remaining part of this section we will argue with the help of further numerical analysis that this is very likely to be the case.

We first investigate for which bands and field values the maximum stretching factor for a fixed q occurs. We observe that the maximum stretching factor always occurs when covering the spectrum for $1/(q+1)$ with the bands of the spectrum for $1/q$. At these magnetic fields the maximum stretching factor stems from the central bands, namely

$$\max_{\substack{p,p',q',i \\ q' \leq 300}} R_i\left(\frac{p}{q}, \frac{p'}{q'}\right) = R_{\left\lfloor \frac{q+1}{2} \right\rfloor}\left(\frac{1}{q}, \frac{1}{q+1}\right), \qquad (18)$$

where $\lfloor x \rfloor$ denotes the integer part of x. For example, in the case $q = 3$ ($q = 4$) the maximum stretching factor occurs when using the second band of $p/q = 1/3$ ($p/q = 1/4$) to cover the cluster containing the second and third band of $p'/q' = 1/4$ ($p'/q' = 1/5$) (Fig. 1). Figure 2 shows $R_{\left\lfloor \frac{q+1}{2} \right\rfloor}\left(\frac{1}{q}, \frac{1}{q+1}\right)$ as a function of q. It has a maximum value of about 2.015 at $q \simeq 300$ and is asymptotically decreasing towards 2, so that it is bounded from above. This behaviour is substantiated (Fig. 2) by using results from Thouless and Tan [29] giving an approximation of the band edges for magnetic fields of the form $1/q$.

Since Hofstadter's butterfly is self-similar, one expects that the stretching factors coming from smaller distorted copies of the butterfly play an important role. In fact, one may wonder if they require larger stretching factors, because of their distortion. For example, such a copy lives between the lowest two bands of $1/3$ and $1/2$ (Fig. 1) with an effective magnetic field σ_{eff} given by $\sigma = 1/(2 + \sigma_{\text{eff}})$. Assuming that in the smaller copies the same bands as in the original butterfly need the largest stretching factors, we investigated the stretching factors of the center bands of this distorted copy for $\sigma_{\text{eff}} = 1/q_{\text{eff}}$ when covering the spectrum for $\sigma'_{\text{eff}} = 1/(q_{\text{eff}} + 1)$. As can be seen in Fig. 2 (crosses) they converge towards the corresponding stretching factors of the original butterfly, however, with deviations for small q_{eff}. A systematic analysis of these deviations also for other small copies of the butterfly shows that these deviations are bounded (Fig. 3). This suggests that Eq. (17) remains valid even without the restriction $q' \leq 300$ and thereby gives strong numerical evidence for the validity of Conjecture 1.

V. CONCLUSION

We have conjectured that the spectrum of the Harper operator for a rational value of the incommensurability parameter σ can be covered by the spectrum for a rational approximant of σ after stretching the bands of the latter by a factor R independent of σ. This factor is numerically found to be $R \approx 2.1$. We showed that from this Conjecture follows that the spectrum is a zero measure Cantor set for *all* irrational σ. Furthermore, it implies that the Hausdorff dimension of these spectra is bounded from above by $1/2$. While these results are for irrational values of σ, the underlying conjecture is stated for pairs of rational values of σ. This allowed a detailed numerical study giving strong numerical evidence for our Conjecture. As we give an explicit construction of the cover used for the conjecture, we hope that our numerical approach is helpful in finding a rigorous proof of these results.

APPENDIX

Here we describe in detail how the cover used in Section IV is constructed using Hofstadter's rules [2,23]. This set of rules describes qualitatively the self-similar structure of the graph in Fig. 1. For a given magnetic field σ the energy spectrum of the Harper operator consists of three non-overlapping parts, one central cluster C and two side clusters L and R. These three parts are distorted Harper spectra for effective field values σ_L, σ_C and σ_R which are given by

$$\sigma_L = \sigma_R = \begin{cases} \left\{ \frac{1}{\sigma} \right\} & \text{for } 0 < \sigma \leq \frac{1}{2} \\ \left\{ \frac{1}{1-\sigma} \right\} & \text{for } \frac{1}{2} < \sigma < 1 \end{cases} \qquad (19)$$

$$\sigma_C = \begin{cases} \left\{ \frac{\sigma}{1-2\sigma} \right\} & \text{for } 0 \leq \sigma < \frac{1}{2} \\ \left\{ \frac{1-\sigma}{2\sigma-1} \right\} & \text{for } \frac{1}{2} < \sigma < 1 \end{cases}, \qquad (20)$$

where $\{x\}$ denotes the fractional part of x. These rules also apply to the distorted spectra such that the spectrum splits into three clusters, each of which splits into three clusters. For irrational σ this splitting is continued ad infinitum. In contrast, for rational σ this process eventually stops for each cluster when it consists of either a single band ($\sigma_{\text{eff}} = 0$) or of two bands ($\sigma_{\text{eff}} = 1/2$); see Fig. 4 for $\sigma = 5/8$. For σ', where σ was obtained by truncating the continued fraction expansion of σ', we simultaneously apply Hofstadter's rules up to the same level as for σ; see Fig. 4 for $\sigma' = 34/55$. This defines a straightforward assignment of a band with $\sigma_{\text{eff}} = 0$ in the spectrum for σ to a cluster of bands in the spectrum for σ'. In the case $\sigma_{\text{eff}} = 1/2$ one has two bands that have to cover the corresponding cluster, which consists of three subclusters. We assign one band to two subclusters and the other band to the third subcluster (Fig. 4) such that the possibly necessary stretching factors for the bands

in order to cover their subcluster are minimized. By this procedure we assign every band of σ to a cluster of bands of σ', where the union of these clusters is the complete spectrum for σ'.

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FIG. 1.   The energy spectrum of Harper's operator [Eq.(1)] for $\lambda = 2$ as a function of the incommensurability parameter σ. The resulting graph is known as Hofstadter's butterfly.

FIG. 2.   Stretching factor $R_{\lfloor \frac{q+1}{2} \rfloor} \left(\frac{1}{q}, \frac{1}{q+1} \right)$ vs. q (diamonds) compared to its analytic value (solid line) obtained from an approximation of the band edges for magnetic fields of the form $1/q$ by Thouless and Tan [29]. The crosses show the corresponding stretching factors of the distorted copy of the butterfly between the lowest two bands of 1/3 and 1/2 (Fig. 1) vs. q_{eff} (see text).

FIG. 3. Maximum deviation $\Delta(\tilde{q})$ of stretching factors in the copies of the butterfly around $\tilde{p}/\tilde{q}$ from the corresponding stretching factors in the original butterfly (diamonds in Fig. 2). Only stretching factors for $1/q_{\text{eff}}$, analogous to $R_{\lfloor \frac{q+1}{2} \rfloor} \left(\frac{1}{q}, \frac{1}{q+1} \right)$ in the original butterfly, are taken into account. For different q_{eff} the maximum is taken over all copies of the butterfly and all $\tilde{p}$. For each q_{eff} the deviations remain bounded and the upper bounds decrease with increasing q_{eff}.

FIG. 4. Assignment of bands in the spectrum for $\sigma = 5/8$ to clusters of bands in the spectrum for $\sigma' = 34/55$ by simultaneously applying Hofstadter's rules. The assignment is straightforward, except for the case $\sigma_{\text{eff}} = 1/2$ where two bands have to be assigned to three subclusters (see text). The arrows mark the cases where bands have to be stretched in order to cover their assigned cluster.

5/8

34/55

L   C   R

2/3   1/2   2/3

13/21   8/13   13/21

L   C   R   L   C   R

0   0   0   0   0   0

5/8   3/5   5/8   5/8   3/5   5/8